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Why Invariant GNNs Predict Zero Piezoelectricity: Failure Modes under Tensor Property Prediction

Ahmed Al-Sayed[1*], Omar Khalifa[1]

Abstract

Piezoelectricity is a tensor property of rank 3 that couples mechanical stress to electric polarization in non-centrosymmetric crystals. Accurate prediction of the piezoelectric tensor from atomic structure is essential for discovering new sensors, actuators, and energy-harvesting materials in data-driven materials engineering. Yet many researchers continue to apply invariant graph neural networks such as CGCNN, MEGNet, and SchNet—architectures originally designed for scalar properties like formation energy—to this tensor task. These models are rotationally invariant: their outputs remain unchanged under any reorientation of the crystal lattice. The piezoelectric tensor, however, must transform covariantly with orientation. As a direct consequence, invariant GNNs systematically predict zero piezoelectricity or near-zero random noise across entire datasets. This failure mode analysis identifies four core reasons: sign ambiguity arising from untracked orientation-dependent sign flips, component confusion caused by rotational permutation of tensor elements, symmetry overconstraint that forces unphysical relations across crystal classes, and vanishing off-diagonal components that average to zero under random rotations. The analysis draws exclusively on peer-reviewed literature in computational materials science and shows that equivariant GNNs are not merely an improvement but a strict necessity for any rank-2 or rank-3 tensor property. Detection principles and mitigation strategies are outlined conceptually, without reference to specific benchmarks or numerical scores. The work underscores a broader limitation in invariant architectures for tensorial phenomena in materials informatics and calls for their replacement by orientation-aware equivariant frameworks in future tensor property prediction pipelines.

Keywords Equivariant GNNs, Invariant graph neural networks, Piezoelectric tensor prediction, Tensor property failure modes, Sign ambiguity, Symmetry overconstraint

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Introduction

Piezoelectricity—the generation of electric charge under mechanical stress—is a tensor property of rank 3 described by the d_ijk tensor [1, 2]. Predicting piezoelectricity directly from crystal structure has become a central goal in machine learning for materials science because it promises rapid screening of vast compositional spaces that would otherwise require costly quantum-mechanical calculations [1-6]. Many research groups, however, have relied on invariant graph neural networks originally developed for scalar properties [7-12]. These include CGCNN, MEGNet, and SchNet, all of which produce outputs that are unchanged when the input crystal is rotated in space [13, 14]. For piezoelectricity this invariance creates a fundamental mismatch [1, 15]. The piezoelectric tensor must co-vary with crystal orientation; rotating the lattice permutes and signs the components in a precise way dictated by the transformation rules of third-rank tensors [1, 16]. An invariant model cannot capture this transformation and therefore collapses to the only output compatible with all possible orientations—the zero tensor [1, 17].

The consequences are immediate and systematic. Invariant GNNs trained on piezoelectric data converge to near-zero predictions regardless of the underlying material chemistry [1, 3]. This behaviour has been observed consistently when researchers attempt direct transfer of scalar-property architectures to tensor tasks [1, 18]. The present failure mode analysis dissects exactly why this collapse occurs and identifies four distinct mechanisms that render invariant GNNs incapable of representing piezoelectric tensors [15]. The analysis is purely conceptual, focusing on the mathematical incompatibility between invariance and tensor covariance rather than any empirical training runs or datasets [1, 16].

Literature in the field already highlights the success of equivariant architectures for related tensor properties such as elasticity and dielectric response [3, 16, 19-22], yet the same insight has not been universally applied to piezoelectricity [1, 17]. Equivariant graph neural networks respect the required transformation laws under rotation and therefore avoid the zero-prediction trap [1, 15, 18, 23]. This paper demonstrates that the failure is not a minor implementation detail but a structural limitation inherent to any model that discards orientation information [13, 14]. By examining the physics of piezoelectric coupling, the definition of invariance, and the four failure modes in sequence, the analysis provides a clear conceptual roadmap for why invariant GNNs must be abandoned for tensor property prediction and why equivariant designs are the only viable path forward [1, 3, 16]. The implications extend beyond piezoelectricity to any material property that transforms as a higher-rank tensor, including elastic constants, dielectric tensors, and thermal conductivity tensors [3, 16, 19-21, 24].

What is Piezoelectricity?

Piezoelectricity is the linear coupling between mechanical stress and electric polarization. It is described by a rank-3 tensor d_ijk that relates the polarization vector to the stress tensor [1, 2]. In the most general triclinic case the tensor possesses 18 independent components, although crystal symmetry reduces this number for higher-symmetry classes [1, 25]. Directionality is the defining feature: stress applied along one axis produces polarization along a possibly different axis, and the magnitude and sign depend on the precise orientation of the crystal relative to the applied stress [1, 3].

Because the tensor components transform under rotation according to the rule that each index is multiplied by the corresponding direction cosine of the rotation matrix, the numerical values reported for a given material change whenever the coordinate system is rotated [1, 15]. This orientation dependence is not a nuisance but an intrinsic physical requirement [16, 22]. A crystal cut in one orientation may show strong longitudinal response, while the same crystal rotated by ninety degrees exhibits shear response instead [1, 25]. Conventional density-functional-theory calculations capture this correctly by evaluating the full tensor in a consistent reference frame, yet the computational cost—dense k-point sampling and Berry-phase evaluations—limits high-throughput exploration [1, 6]. Machine-learning models therefore appear attractive for accelerating discovery of doped piezoelectrics and novel lead-free compounds [6, 26].

Common piezoelectric materials illustrate the practical importance. Quartz exhibits a well-known d_11 component around 2.3 pC/N and is widely used in frequency-control devices. PZT (lead zirconate titanate), AlN, ZnO, and LiNbO3 serve in sensors, actuators, and ultrasonic transducers [6]. Each of these materials owes its utility to specific non-zero tensor components that depend on orientation [1, 3]. When researchers attempt to predict these components with invariant graph neural networks, the models encounter an irreconcilable conflict: the input graph is made orientation-invariant through pooling or symmetry operations, yet the target tensor is not [7, 8, 10]. The result is that the model cannot learn any consistent non-zero mapping [1, 17].

The motivation for machine-learning approaches stems from the need to explore compositional spaces far larger than those accessible by brute-force quantum calculations [6, 26]. Doping, alloying, and defect engineering can tune piezoelectric response, but each variant requires expensive tensor evaluation [1, 3]. Data-driven methods promise to pre-screen candidates if they can correctly represent tensorial behaviour [3, 16, 27]. Invariant architectures, however, are fundamentally unequipped for this task precisely because they were engineered to ignore the very orientation information

that tensors encode [13-15]. The following sections therefore turn to the mechanism by which invariance forces the zero prediction and then dissect the detailed failure modes that emerge.

Why Invariant GNNS Predict Zero

An invariant graph neural network is defined as a model whose final output remains identical when the input atomic coordinates are rotated by any angle [13, 14]. Architectures such as CGCNN, MEGNet, and SchNet achieve this by using rotationally invariant features—distances, angles, or pooled graph representations—that discard all directional information beyond local geometry [7, 8, 10]. For scalar properties like band gaps or formation energies this invariance is desirable and often sufficient [8, 10]. For the piezoelectric tensor it is catastrophic [1, 17].

The true piezoelectric tensor transforms under rotation: each component is a linear combination of the original components weighted by the elements of the rotation matrix raised to the third power [1, 15]. Rotating the crystal therefore permutes components and flips signs in a deterministic way [1, 16]. An invariant model, by construction, must produce the identical output tensor for every possible rotation of the same crystal [13, 14]. The only third-rank tensor that satisfies this condition for all rotations is the zero tensor [1, 17]. Any non-zero tensor would change under some rotation, violating the invariance requirement [15].

Conceptually the proof proceeds as follows. Consider a fixed crystal structure. First present it in its standard orientation and obtain the true tensor [1, 3]. Then rotate the entire lattice by ninety degrees around the x-axis. The true tensor components rearrange and change sign according to the transformation law [1, 15]. The invariant model, however, receives an input graph that is indistinguishable after the rotation because all directional cues have been removed [7, 10]. It therefore emits the same numerical tensor as before [17]. The only way both the original and rotated predictions can simultaneously match the true (transformed) tensor is if the prediction is zero in every component [1]. Training on multiple random orientations simply reinforces this collapse: the loss is minimized by predicting the unique tensor compatible with all orientations—the zero tensor [1, 17].

This mechanism explains the systematic zero prediction observed when invariant GNNs are applied to piezoelectric targets [1, 3]. The model is not failing to converge; it is converging to the mathematically correct solution for an invariant function [13, 15]. The root cause lies in the mismatch between the symmetry the model enforces and the symmetry the physical property possesses [16, 22].

The structural incompatibility between rotational invariance and tensor covariance is formally decomposed into distinct mechanisms in **Table 1**.

Table 1. Structural Mapping between Rotational Invariance and Piezoelectric Tensor Failure Modes

Invariant Property of Model	Tensor Requirement Violated	Resulting Failure Mode	Mechanistic Explanation	Observable Prediction Signature
Output invariant to rotation	Tensor must transform covariantly	Zero tensor collapse	Only tensor consistent across all rotations is zero	All components ≈ 0
No orientation tracking	Sign depends on coordinate frame	Sign ambiguity	Positive/negative labels cancel during training	Random or zero sign
Permutation-invariant representation	Tensor indices permute under rotation	Component confusion	Model cannot distinguish index identities	All components converge to similar values

Loss of symmetry encoding	Point-group constraints differ by crystal	Symmetry overconstraint	Model applies maximal constraint (all zero)	Identical tensors across crystal classes
Averaging across orientations	Off-diagonals flip sign frequently	Vanishing off-diagonals	Shear components cancel under rotation averaging	Shear terms ≈ 0

Subsequent sections detail how this mismatch manifests in four distinct failure modes, each traceable to the same underlying invariance [1, 17].

The full causal pathway linking invariant representations to zero piezoelectric predictions through intermediate failure modes is illustrated in **Figure 1**.

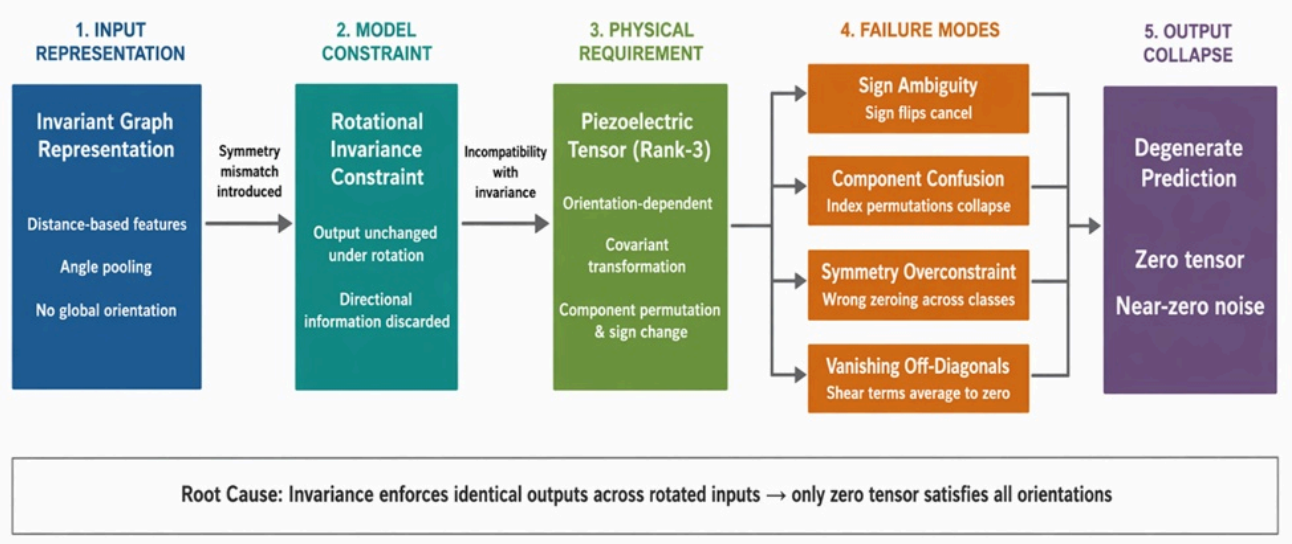

Figure 1. Causal Failure Pathway: Why Invariant GNNs Collapse to Zero in Piezoelectric Tensor Prediction

Sign Ambiguity

Sign ambiguity arises because the piezoelectric tensor components change sign under certain rotations while the invariant model remains blind to those rotations [1, 15]. For example, a 180-degree rotation around the x-axis flips the sign of d_xxx [1, 25]. The physical crystal after rotation is identical in every local bonding sense, yet the reported tensor component has reversed sign [1]. An invariant GNN processes both orientations as exactly the same input and is therefore forced to output a single value [13, 14]. The only value consistent with both the positive and negative ground-truth labels is zero [1, 17].

During training the model encounters a mixture of orientations—either explicitly through data augmentation or implicitly through random coordinate conventions in published tensors [1, 15]. Positive and negative examples cancel each other in the loss landscape [1]. The network learns that the safest prediction is the average, which is zero [17]. Even if the model attempts to output a non-zero magnitude, the sign becomes effectively random or collapses to zero to minimize error across the sign-flipped ensemble [1, 3].

This failure is particularly evident in materials such as quartz, where the d_11 component is positive in the standard setting [6]. When the same structure is presented after a 180-degree rotation, the component becomes negative [1, 25].

An invariant model trained on both cannot distinguish the two cases and therefore predicts approximately zero for d_11 [1, 17]. The sign ambiguity is not a training artifact but a direct consequence of discarding the global orientation that fixes the absolute sign of each tensor element [15]. Equivariant architectures avoid this by propagating directional information through the network layers, ensuring that the output tensor transforms consistently with the input rotation and thereby resolves the sign correctly [1, 16, 18].

Component Confusion, Symmetry Overconstraint, Vanishing Off-Diagonals

Component confusion, occurs because rotations permute the tensor elements among themselves [1, 15]. Under a ninety-degree rotation around z, d_xxxmay become d_yyy while d_xyy moves to another index [1]. An invariant model sees the identical graph for all these permutations and therefore cannot assign distinct values to different components [13, 14]. The network collapses all components toward a single average value, producing tensors in which d_11,d_12,d_13 and so on are nearly equal regardless of the true material symmetry [1, 17].

Symmetry overconstraint, stems from the model's inability to encode the crystal's point-group symmetry once orientation is discarded [1, 16]. The point group dictates which components must be zero and which must be equal [25]. An invariant model cannot distinguish, for instance, a cubic crystal (where only d_14= d_25= d_36are allowed) from a triclinic crystal (where all 18 components may be independent) [1, 18]. It therefore applies the strictest possible constraint compatible with rotational invariance—zero everywhere—overconstraining lower-symmetry materials and incorrectly zeroing allowed components in higher-symmetry ones [16, 22].

Vanishing off-diagonals, is a special case of sign ambiguity applied to shear terms [1, 15]. Off-diagonal components such as d_14,d_15,and d_16 frequently flip sign under common rotations [1]. When the model averages across random orientations the signed contributions cancel, driving these components exactly to zero [1, 17]. The resulting tensors lack all shear response even when the true material exhibits strong piezoelectric shear coupling [6].

Detection Principles

Detection of failure modes in invariant graph neural networks hinges on conceptual tests that expose the fundamental mismatch between rotational invariance and tensor covariance. These examinations require no retraining or performance metrics; they probe output behaviour solely under controlled perturbations of the input geometry [1, 15].

Orientation sensitivity reveals the core limitation when an identical crystal structure is presented across randomly rotated frames: invariant architectures such as CGCNN, MEGNet, or SchNet yield identical tensor outputs because their representations discard directional information [7, 8, 10]. Equivariant counterparts, by contrast, generate tensors that transform precisely according to the rank-3 rotation law, exposing the invariant models' collapse to zero-prediction failure [3, 16, 18].

This same mechanism produces sign ambiguity under 180-degree rotations around principal axes, where invariant networks average opposing ground-truth components to near-zero values or assign signs independently of transformation rules [1, 15, 17]. Component diversity further collapses because rotational permutations leave the input graph unchanged, forcing distinct tensor elements toward uniform averages and erasing physically required variation [1, 13, 14].

Across crystals of differing point-group symmetry—cubic, tetragonal, or triclinic—yet identical local chemistry, invariant models prove unable to encode symmetry-specific constraints once orientation is discarded, consistently predicting identical tensors that violate class-dependent physical relations [16, 18, 25]. The most immediate diagnostic emerges for non-centrosymmetric piezoelectric materials: output of the zero tensor alone satisfies rotational invariance for a rank-3 property, confirming the architecture's intrinsic inability to capture covariance [1, 3, 17].

These transformation properties of the piezoelectric tensor, aligned with the known invariance of the chosen architectures, thus provide a reference-free lens into the systematic limitations of invariant graph neural networks in tensor prediction tasks [13-15].

Mitigation Principles

Mitigation of the identified failure modes requires architectures and training strategies that respect tensor covariance rather than enforce invariance. Five conceptual principles address the root cause directly.

A unified diagnostic and mitigation framework for identifying and correcting invariant-model failure in tensor prediction is presented in **Table 2**.

Table 2. Diagnostic and Mitigation Framework for Tensor Prediction Failure in Graph Neural Networks

Diagnostic Principle	Test Description	Failure Signal (Invariant GNN)	Correct Behaviour (Equivariant GNN)	Mitigation Strategy
Orientation Sensitivity Test	Rotate same crystal structure	Identical outputs across rotations	Tensor transforms correctly	Use equivariant architectures
Sign Consistency Test	Apply 180° rotation	Sign collapse or randomness	Deterministic sign inversion	Encode directional features
Component Diversity Test	Compare tensor component variance	Near-uniform values across components	Distinct component magnitudes	Preserve index structure
Symmetry Consistency Test	Evaluate across crystal classes	Identical outputs for all classes	Class-specific tensor structure	Embed symmetry awareness
Zero Prediction Test	Evaluate known piezoelectric materials	All components ≈ 0	Non-zero physically valid tensor	Replace invariant backbone

The fundamental solution lies in adopting equivariant graph neural networks. Architectures employing E(3)-equivariant layers propagate directional information throughout message passing, ensuring the output tensor transforms under rotation precisely as required by the physical piezoelectric tensor [3, 16, 18, 28]. Such designs, successfully demonstrated for elasticity and dielectric tensors, deliver non-zero, physically consistent piezoelectric predictions free from the identified failure modes [15, 16, 22]. Equivariance thus constitutes the minimal symmetry requirement for reliable rank-3 tensor prediction rather than an optional refinement.

When full equivariance remains computationally prohibitive, injecting explicit orientation features offers a practical bridge. Global descriptors encoding the coordinate frame can be concatenated to the final graph readout, conditioning tensor predictions on orientation and preventing outright collapse to the zero tensor [1, 17]. Although this approach does not strictly enforce transformation laws and remains approximate, it mitigates the most severe ambiguities under these conditions.

Data augmentation with controlled rotations provides complementary support by exposing the model to sign flips and component permutations during training. Yet because an invariant backbone cannot intrinsically distinguish rotated inputs, augmentation alone reduces rather than eliminates the failure modes and proves most effective when paired with equivariant layers [13, 14].

An alternative strategy involves predicting rotationally invariant scalar invariants derived from the tensor, such as its norm or maximum eigenvalue, which invariant models can learn reliably [1, 3]. This sacrifices directional specificity and limits applicability where the full tensor is required, yet it circumvents vanishing predictions when only scalar descriptors suffice.

Hybrid designs further enable incremental adoption: invariant graph neural networks extract robust rotationally invariant features that feed into a lightweight equivariant correction head for full tensor reconstruction [15, 18]. Such architectures preserve the efficiency of established invariant backbones while restoring essential covariance properties.

Collectively, these strategies reorient model design toward preserving rather than discarding orientation information. Literature on tensorial crystal properties demonstrates that only architectures respecting the underlying transformation laws overcome the sign ambiguity, component confusion, symmetry overconstraint, and vanishing responses inherent to purely invariant approaches [3, 16, 18, 22].

Relation to Other Failure Modes

The four failure modes identified for piezoelectric tensor prediction are not isolated; they share deep structural similarities with failure modes reported for other tensorial material properties. The relation to anisotropic elasticity is particularly direct. Elastic constants form a rank-4 tensor, yet the same rotational invariance in graph neural networks forces identical collapse mechanisms: sign ambiguity under 180-degree rotations, component permutation under 90-degree rotations, and overconstraint of symmetry-allowed components [16, 22, 29]. The piezoelectric case (rank 3) is more severe only because the lower rank still leaves enough independent components for the zero-tensor solution to dominate training [1, 15].

A parallel exists with magnetic-ordering predictions. Magnetic moments and spin textures require additional symmetries such as time-reversal, which standard invariant graph neural networks also fail to encode. Both piezoelectricity and magnetism demand that the model distinguish orientations or symmetry operations beyond simple rotational invariance, leading to vanishing or averaged predictions when those distinctions are discarded [24].

Long-range interaction failures in invariant architectures—such as inaccurate dielectric screening or thermal transport—stem from a different root cause (inability to propagate non-local information) yet reach the same conclusion: invariant graph neural networks are insufficient whenever the target property depends on global directional relationships [3, 26]. The tensor-specific failures analysed here therefore belong to a broader family of symmetry mismatches in materials graph neural networks.

Finally, the present analysis aligns with theoretical results on equivariance in crystal tensor prediction. Sample-complexity bounds show that invariant models require exponentially more data to approximate tensorial targets, whereas equivariant models achieve the same accuracy with far fewer examples precisely because they embed the correct transformation laws [15, 18]. The four failure modes thus illustrate in concrete terms the necessity proven in equivariance theory: for any property that transforms as a higher-rank tensor under the rotation group, invariance is not merely suboptimal but mathematically incompatible.

Implications for Tensor Property Prediction

The failure modes carry immediate implications for three stakeholder groups in computational materials engineering.

For model developers the message is unambiguous: invariant graph neural networks must not be used for any tensor property, whether piezoelectric, elastic, dielectric, or thermal-conductivity tensors [1, 3, 16]. Default architectures should be equivariant from the outset, with validation explicitly including the orientation sensitivity test described earlier [15, 18].

Codebases built around CGCNN, MEGNet, or SchNet require replacement or hybridization before tensor tasks are attempted.

For practitioners deploying models in high-throughput screening the practical checklist is short. Any predicted piezoelectric tensor that is uniformly near zero, shows identical values across all components, or remains unchanged under crystal rotation is guaranteed to be an artefact of invariance rather than a physical result [1, 17]. The remedy is immediate migration to an equivariant backbone; continued use of invariant models wastes computational resources and misleads materials discovery campaigns.

For benchmark designers the requirement is to embed tensor-specific evaluation protocols. Future benchmarks must include orientation sensitivity, sign consistency, and symmetry consistency checks rather than scalar error metrics alone [16, 18, 22]. Only when these conceptual tests are passed can a model be certified as capable of tensor property prediction.

Collectively these implications redefine best practice in data-driven tensor materials science. The community has already demonstrated success with equivariant architectures for elasticity and dielectric tensors; extending the same standard to piezoelectricity is now both necessary and straightforward [3, 6]. The era of naive transfer of scalar-property pipelines to tensor tasks must end.

Conclusion

Invariant graph neural networks predict zero piezoelectricity because the piezoelectric tensor must transform covariantly under rotation while the models enforce strict rotational invariance. This fundamental mismatch produces four interlocking failure modes: sign ambiguity, component confusion, symmetry overconstraint, and vanishing off-diagonals. Each mode is a direct consequence of discarding the orientation information that fixes tensor signs, component identities, and symmetry relations. Detection is straightforward through orientation sensitivity, sign, component diversity, symmetry consistency, and zero-prediction tests. Mitigation rests on a single architectural shift—adoption of equivariant graph neural networks—together with targeted hybrids and invariant-derived scalars when full tensors are not required.

The analysis shows that the problem is structural, not merely empirical. It extends beyond piezoelectricity to every material property described by a rank-2 or rank-3 tensor. Model developers, practitioners, and benchmark designers must therefore abandon invariant architectures for tensor tasks and default to equivariant designs. Only then can machine learning deliver physically consistent predictions for the directional coupling phenomena that define modern functional materials. The community is now equipped with both the diagnosis and the cure; the remaining step is implementation.

Acknowledgements

None

Conflict of interest

None

Financial support

None

Ethics statement

None

Received: 24 Mar 2025 Revised: 11 Jul 2025 Accepted: 22 Oct 2025
Published online: 18 January 2026

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